Artificial intelligence and virtual environment application for materials design methodology

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ABSTRACT

Purpose: The purpose of this study is to develop a methodology for material design, enabling the selection of the chemical elements concentration, heat and plastic treatment conditions and geometrical dimensions to ensure the required mechanical properties of structural steels specified by the designer of machinery and equipment as the basis for the design of material components manufactured from these steels, by using a computational model developed with use of artificial intelligence methods and virtual environment. The model is designed to provide impact examinations of these factors on the mechanical properties of steel only in the computing environment.

Design/methodology/approach: A virtual research environment built with use of computational model describing relationships between chemical composition, heat and plastic treatment conditions and product geometric dimensions and mechanical properties of the examined group of steel was developed and practical applied. This model enables the design of new structural steel by setting the values of mechanical properties based on material production descriptors and allows the selection of production descriptors on the basis of the mechanical properties without the need for additional tests or experimental studies in reality.

Findings: Virtual computing environment allows full usage of the developed intelligent model of non-alloy and alloy structural steel properties and provides an easy, intuitive and user-friendly way to designate manufacturing descriptors and mechanical properties for products.

Research limitations/implications:The proposed solutions allow the usage of developed virtual environment as a new medium in both, the scientific work performed remotely, as well as in education during classes.

Practical implications: The new material design methodology has practical application in the development of materials and modelling of steel descriptors in aim to improve the mechanical properties and specific applications in the production of steel. Presented examples of computer aid in structural steel production showing a potential application possibility of this methodology to support the production of any group of engineering materials.

Originality/value: The prediction possibility of the material mechanical properties is valuable for manufacturers and constructors. It ensures the customers quality requirements and brings also measurable financial advantages.

Keywords: Materials science virtual laboratory; Artificial intelligence methods; Computational material science and mechanics; Iron alloys metallurgy

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RESEARCH MONOGRAPH

1. Introduction

The increasing consumer demands about better quality of steel products forcing on manufacturers the usage of more precise manufacturing processes, which are based on the rigorous standards. To stay on the market, it is necessary to use computer systems supporting steel production or project managing on each stage of manufacturing. Increase in computing power, observed in recent years, favours the development of modern tools used for improving of product quality or for lowering its price. On special attention deserves, developed for several years, computer systems based on artificial intelligence methods and used to predict the mechanical properties of manufactured material. These systems absolving manufacturers from the multiple repetitions of expensive and long-term laboratory researches. The ability of structural steels mechanical properties obtainment is extremely valuable for manufacturers and designers, which are manufacturing or using steel elements. This allows fulfilling all customers' requirements regarding the quality of supplied products. Modelling of steels mechanical properties is also associated with financial benefits, when expensive and time-consuming researches are reduced to necessary minimum. Necessary to conduct is only the verification of computations. Material science research centres for several years are engaged in intensive researches to develop computational models applicable to determination of the mechanical properties. Such model, with are providing a comprehensive modelling of the steels mechanical properties, has not been developed yet. There are many computational models described in the literature, which can be used for predicting the mechanical properties of different materials, but their usage in industry is limited because of narrow ranges of chemical composition or specific production conditions [1-4].

This situation forced to develop a new computational model covering a wide range of input values, such as the high number of chemical elements, treatment conditions and geometrical dimensions, and relate them with the greatest possible number of mechanical properties. Suitable tools developed for modelling facilitation of these properties will enable more effective selection of steel production descriptors. It will also enable manufacturing of higher quality product, which are cheaper and are more optimized for customer needs. The development of computational methods and computer simulations resulted in replacement of the traditional laboratory in favour of the virtual laboratory. Development of virtual tools, which are simulating the investigative equipment and simulating the research methodology, can serve as a basis for combining aspects of laboratory research, simulation, measurement, and education. Application of these tools will allow the transfer of research and teaching procedures from real laboratory to virtual environment. This will increase the number of experiments conducted in virtual environment and thus, it will increase the efficiency of such researches. This will also allows the training of more professionals. This is not the work on real hardware. This is work with use of suitably designed simulators, namely those, in which the real research methodology

is faithfully reproduces. Such simulators are very helpful, not only in industrial applications, but also in engineering education. Such researches were already preformed in the Department of Materials Processing Technology, Management and Information Technology in Materials Institute of Engineering Materials and Biomaterials, but this was not an integrated and comprehensive approach. Presented in this paper the new approach allows the methodical use of all available computational techniques, including the artificial intelligence tools and virtual environment [4-6].

2. A literature review

2.1. The usage of IT tools in the design of material products

The aim of new engineering materials design is to optimize their functional properties in technological, economic and environmental aspect. This usually applies to products made from these materials, which meet the strict usage requirements. Such design, usually computer aided, must be based on a thorough knowledge of relations (theoretical and empirical) between the chemical composition of the material, its structure, treatment conditions and mechanical properties. The main benefit is the ability to design a suitable material selection (or manufacturing) methodology for various industrial applications [7-9]. The idea of modelling is shown in Figure 1.
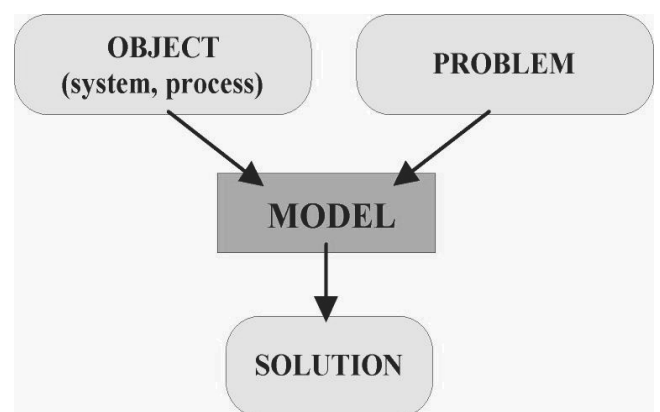

Fig. 1. The idea of modelling

Models shall be construed as a reflection of the system with use of logical relationships between variables describing them. Manipulation of these variables allows the analysis, how the model behaves in certain conditions [10]. Computational model is a simplified description of the relation between steels mechanical properties and conditions of its production. It ignores certain dependencies occurring in reality (considered by model developers to be less important) [8,11-13].

Evaluation of simulation results obtained with use of developed computational model is based on comparison of all relevant variables model with the measured data [14-15]. It is recommended when developing a model to obtain a comparable level of the representation accuracy for most variables than the unusually precise terms of one variable (although important), and poorly to others [16-19].

Computational material models are collections of information on their properties and descriptors, expressed as a mathematical equation. Modelling is thus formalizing the description methodology of the given property, limited to set of properties shown by the physical model with use of formulas and mathematical relationships. This means that the physical model determines the form of a mathematical model. The mathematical model should clearly correspond to the physical model [20-23].

2.2. Numerical and mathematical models of structural steels

There are many techniques of mathematical modelling using several different algorithms described in available literature. They are used among others to modelling the steels mechanical properties. The popularity of structural steels is very big. This type of steel is also very well described in the literature. Looking through libraries and internet resources a huge number of works can be found, which are describing every steel property in detail, not only about mechanical properties. Equally large is collection of articles and books related to properties' modelling, from the simple dependence equations, through statistical analyses and on the methods of artificial intelligence finishing [12-15].

However, there is no universal method of mechanical properties prediction. Developed and described in the literature models can be applied in very limited range of the chemical elements concentration or even for single steel grade with very narrow manufacturing conditions. Some part of all models does not take into consideration important conditions as e.g. the production focusing exclusively on the chemical composition on maximum four alloy additions

The majority of models are developed to modelling exclusively single, chosen mechanical property. Another difficulty, which can occur while modelling, is the complete abstraction of models, which are based exclusively on theoretical dependencies without using of real data coming from real material investigations. Such models, sometimes very complex, are not describing real conditions very well. They are too idealised and they are not taking into consideration many important factors present during the production. It is hard to apply such models in industry conditions.

Numerous examples of equations, which are used most often to calculate the yield strength or tensile strength on the basis of the chemical elements concentration or on the treatment parameters, can be also found in literature. These examples are however only simple approximations of large data sets and are not determine the property with satisfactory exactitude.

Empirical examples, made with use of the statistical analysis of the real investigation results, also deserve for the attention. These examples, however, can be applied only when the steel type is strictly defined (with very narrow ranges of describing factors) and only when the steel was developed in precisely definite environment. This is not always possible in industrial conditions [16-19].

2.3. Application of artificial neural networks in the construction of model

The name "artificial neural networks" describes the hardware or software simulators, which realize semiparallel data processing. They are constructed from many joined neurons and they are imitating the work of biological brain structures.

Application of artificial neural networks considerably simplifies the modelling methodology. There is no need to know the function of input and output parameters in explicit form. If only such function exists, it will be established by the network during the training process and its parameters will be written down as weights values of every individual neuron. The most important thing is that this function exists and has the regular and unique character.

Creation of model with utilisation of artificial neural networks is indicated all there, where the precise physical and mathematical description of the considered phenomenon is not known and where input and output values in descriptive vectors are well determined. Artificial neural network is able to learn how to recognise the analysed problem and it will quickly give the answer on the changing input parameters of the given problem.

In most cases the failure of neural network creation is caused by the lack of the assignment function (output parameters are independent from input parameters) or the function is strong deformed by the noise, present in descriptive vectors [20-23,78-79].

2.4. Virtual laboratories methodology in scientific researches and education

Virtual laboratory is, located in virtual environment, set of simulators and trainers, whose main objective is to simulate the research methodology of investigative equipment located in real scientific laboratory. Additionally, user can find manual instructions of equipment usage, real and virtual experiments descriptions, training exercises possible to perform and many other materials supporting the cognitive processes of research methodology. Virtual laboratory is among other, training environment for staff and students who have just started work with the given device type. They can acquire basic skills and abilities to operate the device without worrying about damaging

expensive equipment or causing danger to life or health of their own and other peoples present in the lab. Improper handling of simulated device ends only on the simulated malfunction or damages, visible only on the monitor screen. Then, user simply needs to reset the simulation to the initial state and repeat the experiment with the introduced correct parameters. Figure 2 show the concept of a virtual laboratory.

The economic aspect is also very important. Virtual laboratory is extremely cheap to maintain and operate. Except the activation costs, which are covering the preparation of necessary computer system, the implementation of virtual simulation and equipment necessary for their use, present are only the maintenance costs during operation. There is no need of preparation of any materials samples or other supplies, which are sometimes very expensive. Technical inspection of machinery are not necessary, any simulated damage can be eliminated by resetting the simulation to the initial state.

Researches conducted in academic centres indicate that the ability to perform the experiment at home without supervisor has a positive effect on the student. He don't feel helpless and he doesn't make as many mistakes as a student familiar only with the theoretical descriptions of machines and having a first contact with the real device only in the classroom under the supervision of an instructor leading the subject [24-34].
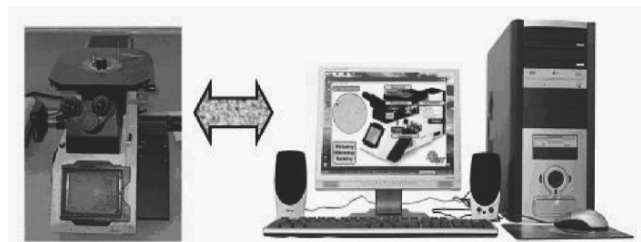

Fig. 2. The concept of a virtual laboratory: replacing of real investigative equipment with virtual simulations

Five postulates of virtual laboratories construction have been developed [23-25,36-38]:
1. The postulate of equality - each student should have access to the same teaching materials. You can not favour students by giving more authority to them, or, opposite, restrict their ability to work in the laboratory,
2. The postulate of availability - each student should have access to a laboratory with the same authority. It should not matter what equipment or what software he use, the system should be accessible anytime from anywhere.
3. The postulate of simplicity - do not extend unnecessary laboratory infrastructure. The interface is an addiction and not the essence of the laboratory. Most important are simulations intended to be simple and understandable because students without adequate knowledge shouldn't have problems in understanding the operating principles of the real equipment,
4. The postulate of representativeness - simulated device or phenomenon should faithfully reproduce their prototypes found in the real world. Everything has to be simulated

exactly as it is in reality. Any changes in the facts are not acceptable.
5. The postulate of openness - the laboratory should allow the easy expansion with new elements, such as teaching materials and simulation. Expansion should be possible for all users of the laboratory.

These postulates shows, that programs, which are simulating real investigative equipment must faithfully represent research methodologies of their real equivalents. Student should learn in a simple and affordable way the usage methodology of investigative equipment, which he will operate in the real world and about which at present time does not have enough information. This should be done regardless of the hardware and software, which is available and regardless of time and place of students' current residence. If the simulation will be difficult to handle or if it will not reflect the simulated machine functionality, it will not have high educational value and it will discourage the work. Similarly, too high hardware requirements can make the study difficult to students, which have an insufficient computer configuration.

It is obvious that the simulator will never reach the full functionality of a real device. The simulator is only a simplified model, which reflects only the basic functions necessary to begin working with a machine. These functions should be placed accurately, because of their cognitive character. Even the best-featured virtual laboratory will never replace the real laboratory. These systems should not be treated as equal. Virtual laboratory should not be substitution for real laboratory. Real and virtual technologies used together offer more opportunities for base training and education than used independently of each other [26-27, 31, 34-35, 39-47].

There are many applications of virtual environment in engineering, starting from simple simulations [48-54], through the virtual design and manufacturing [55-61], and on the entire virtual factories ending [62-66]. Virtual Laboratory depending on the architecture can be defined in several ways.

Application virtual laboratory is a software tool developed to simulate the phenomenon of the device directly on user's computer (Fig. 3). This is software, which must be installed on herd disk. Connection to the Internet is not necessary [67-69].
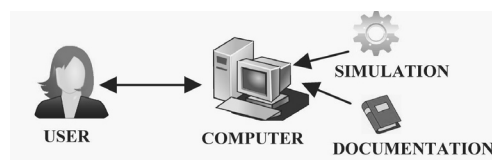

Fig. 3. Architecture of application virtual laboratory

Network virtual laboratory use user's computer as access terminal for to data and simulation placed on the remote server (Fig. 4). In addition, all experiments carried out on simulators are performed on the fast and efficient network server. Only results of virtual researches are passed to the user. This is the most complex architecture of a virtual laboratory, because in

addition to the work of the simulation provides access to other facilities, such as teaching aids, updated academic or technical manuals, support instructors etc. Communication and exchange of data and experiences among participants of virtual courses is also possible. In contrast to the application laboratory, the installation of whole environment onto the hard disk is not required. Necessary are only minor extensions installed in web browser to allow two-way communication with the server and display of the virtual content on the user monitor screen [67-69].
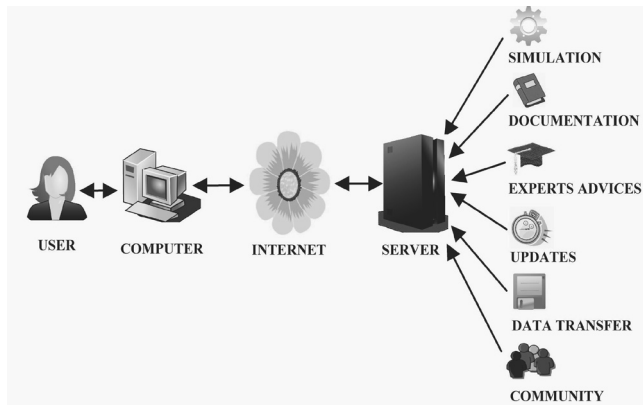

Fig. 4. Architecture of network virtual laboratory

Remote access virtual laboratory is not virtual in the literal sense. This is a real laboratory (consisting of real objects), that can be controlled remotely over internet (Fig. 5). Video transmission is carried out from the bench to the user using a web camera, connected with data server. The start of the experiment in this type of laboratory is a big disadvantage. In most cases, operator intervention is required in place of the experiment. To build a fully automated workroom is possible only for very simple systems. For more complex laboratory, automation costs are disproportionate to the achieved results. In the case of remote controlled laboratory, it is not possible to access the device by more than one user at the same time. In addition, delays in transmission of data between the user and the device can have a disastrous impact on the experiment progress. This is very important, particularly, where prompt decisions are critical in achieving of success in researches [67-69].
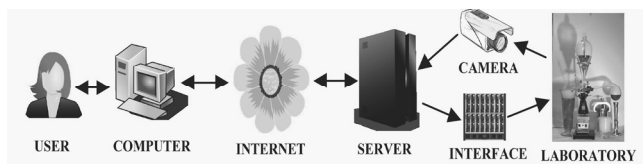

Fig. 5. Architecture of remore access virtual laboratory

3. Course and range of own work

3.1. Research scope

In order to accomplish the main objective of this work, namely to develop a computer-aided method of steel mechanical properties modeling with use of artificial inteligence tools and virtual environment and links them to the chemical composition, conditions of heat and plastic treatment and geometric dimensions of product, materials research were carried out in order to build a database of experimental results, which was then used in the training process of artificial neural networks. This database was used to build a computational dependences model based on structural steels. To take full advantage of the developed computational model a materials science virtual laboratory was designed, developed and then used to predict the mechanical properties of the structural steels and to visualization of modelling results. It is placed in virtual reality an open science, research, simulation and teaching environment, which enable researches on selected mechanical properties of structural steels. Verification researches were performed to confirm the efficiency of virtual environment application for the purpose of modelling, simulation and prediction of mechanical properties of engineering materials on the example of structural steel on the basis of descriptors such as chemical composition, heat and plastic treatment conditions and shape and dimensions of the product. Developed software and obtained experimental results were used to work on the modelling of production conditions of non-alloy and alloy structural steel meeting the requirements specified by the designers of machinery and equipment. Possible are also classes on science research methodology and operation of research equipment for students and young engineers carried out by use of traditional and e-learning methods.

3.2. Material and research methodology of structural steels mechanical properties

Non-alloyed and alloyed structural steels were selected for examinations as example material. As the main criterion for selection of steel types was the carbon concentration, which for structural steel does not exceed 0.6% [70-71]. Further criteria for minimal and maximal chemical elements concentration, conditions of heat and plastic treatment were taken from [93] and [94]. The selection of mechanical properties, which were examined was based on [95] and on analysis of the steel markets [80-88] and study the literature [7, 12, 72-76].

For the description of structural steel, six mechanical properties present in the metallurgical certificate have been selected. To describe the above properties set of descriptors characterizing steel in manufacturing process has been developed. It consists of chemical composition described by concentration of thirteen of the most common elements in steels, two technologies of heat treatment used in manufacturing, two technologies of

plastic treatment and the geometric dimensions of the final product. Steel was manufactured in electric arc furnaces with devices for steel vacuum degassing (VAD). The material was supplied in the form of heat and plastic treated long rods.

Steel samples for the chemical composition examinations were taken from finished products in accordance with [96]. Samples for the static tensile examinations were taken from the rods in accordance with [97]. Measurements of the yield strength, tensile strength, relative elongation and relative area reduction were performed in accordance with [98] on round samples with a diameter of φ10mm and the length of 50mm with use of universal tensile machines ZD-40 manufactured by VEB Leipzig and Amsler FM2750 manufactured by Amsler/Wolpert GmbH. Measurements of the impact strength were made in accordance with [99] on samples with dimensions 10x10x50mm with incised notch in the shape of the V and U letters with a depth of 2mm, on Charpy hammer PSW-300 manufactured by MFL Systeme GmbH and Amsler RKP450 manufactured by Roell-Amsler GmbH. Brinell hardness measurements were performed in accordance with [100] on B1-9TB universal hardness tester manufactured by Łucznik-Radom. Vickers hardness measurements were performed in accordance with [101] on Zwick ZHR hardness tester manufactured by Zwick. All examinations of the mechanical properties were performed under laboratory conditions at room temperature (20° C).

3.3. Description of own work methodology for prediction and modelling of examined structural steels mechanical properties

The set of vectors, which was used for training of artificial neural network, has been collected and developed during the examination of hundred thirty-five structural steels types. These steels were produced in one of the Polish steel plants. Data covering 14212 input vectors were collected. These vectors contain the geometric data of rods, concentration of chemical elements and the conditions of heat and plastic treatment. For each of the input vectors output vector containing a set of mechanical properties modelled values were compiled.

The set of all vectors were divided into three subsets in relation 2-1-1. With half of all vectors a set of vectors used to modify the neuronal network weights (training set) were created, one quarter of vectors was assigned to evaluate the prediction error during learning process (validation set), and the remaining part was used to independent determination of the prediction accuracy at the end of the network training process (testing set). Assignment of vectors to the appropriate sets was random. The required accuracy of prediction is different in different applications. Based on literature data [77-78] was assumed that deviation ratio equal or lover to 0.1 indicates a very good implementation of the regression in the network, while the ratio value equals to 0.7 of above will disqualify the created by the network model. Values from the range of 0.1 to 0.4 are typically obtained values of parameters for modelling of

physical phenomena and engineering values. Regression statistics are determined independently for the training, validation and testing sets. Nature of the problem was defined as standard. Each vector was examined independently of the others. Researches for the best artificial neural network for regression issues were narrowed to structures such as:

- linear neural networks (LNN),
- radial base functions (RBF),
- general regression neural network (GRNN),
- multi layer perceptrons (MLP).

For classification problems following neural network structure were selected:

- linear neural networks (LNN),
- probabilistic neural network (PNN),
- multi layer perceptrons (MLP).

The training process was conducted with use of these algorithms:

- error back propagation,
- conjugate gradient,
- Quasi-Newton,
- Levenberg-Marquard,
- fast propagation
- delta-bar-delta.

To verify the neural network usability for the prediction and modelling purposes regression statistics such as:

- average absolute error,
- standard deviation ratio,
- Pearson R correlation

were used. For quality evaluation of the artificial neural network, implementing the classifications the percentage rate of correct responses related to the size of the network set was determined. All calculations were performed using Statistica Neural Network developed by Statsoft [89].

Developed artificial neural networks were used to build the computational dependency model in structural steel. To build such model forty-nine artificial neural networks were trained. This model was built to verify the correctness of networks' training process and to enable the effective usage of artificial neural networks for prediction and modelling of structural steels properties. The model describes the relationships, which exist between the conditions of steel production and its mechanical properties after manufacturing. After passing into models' inputs the input parameters, which are:

- in case of straight modelling - chemical composition, head and plastic treatment conditions and geometrical dimensions,
- in case of reversed modelling - mechanical properties.

These values are transferred into active block in the computation model. There, these values are distributed simultaneously on all artificial neural networks. Complete results, namely:

- in case of straight modelling - values or ranges of materials properties,
- in case of reversed modelling - concentrations of chemical elements, conditions of heat and plastic treatment or geometric dimensions,

are transferred outside of the model through the user interface. This model was, in the next step, used to build a materials

science virtual laboratory. In application part of the laboratory, developed model is used in direct determination of the descriptors or properties of examined steels. In the network part on the basis of achieved results, the virtual sample file is generated. This file is a representation of real material sample in virtual environment. To obtain the results from this file it should be examined with the use of investigative equipment simulators, like a real material sample.

In order of experimental verification of the developed computational dependency model, a dozen types of non-alloy and alloy structural steels for different purposes were selected for examinations. Comparative studies were conducted using the material science virtual laboratory and real laboratory of the Institute of Engineering Materials And Biomaterials. A set of files describing the conditions of production and mechanical properties of selected species and corresponding to them real, material samples taken from the ready-made steel rods were developed. At model inputs, the production conditions of steel were inputted. Obtained computational results were compared with those obtained by real examinations of real samples of steel material.

The results obtained during examination of real steel were introduced into the material science virtual laboratory. Results obtained in virtual environment were compared with results obtained in real investigations. Computations were conducted independently for all tested steel types.

The chemical composition, treatment conditions and product sizes were also inputted into generation panel of samples in the network laboratory. The results of these actions are the files of steel materials samples. Hardness, impact strength and tensile examinations of generated virtual samples were performed using equipment simulations located in the virtual materials examination laboratory. Observations of steel structure were made in the virtual structure examination laboratory.

Based on the simulation data graphs showing the impact of the steel descriptor on the selected mechanical property of steel was developed. In the appropriate panel of NeuroLab application, production conditions among with the steels property with an appropriate range of variability were inputted. Effect is a graph showing the relationship:

$$y = f(x, z_1 \dots z_n)\Big|_{x_0}^{x_1} \tag{1}$$

where:
    y - value of the property
    x - value of the descriptor
    x_0 - x_1 - the range of variability of the descriptor
    z_1 - z_n - values of all remaining descriptors.

In both parts of the materials science virtual laboratory for modelling of steel's mechanical properties the same computational model based on artificial neural network were used. That means that results obtained in the network part of the laboratory are identical with those obtained from the NeuroLab application. A file, which describes the material

sample developed and used during the work in the network part of the laboratory, can be used in the application part without any modification.

Operations performed in order to design new type of steel were made. Designed new steel should fulfil all strict requirements given by the customer in terms of production conditions and mechanical properties. New steel types were developed with use of material science virtual laboratory as material sample files, which are describing new types of steel meeting all requirements in virtual environment. In order to verify the correctness of performed simulations new steel types were manufactured in real world. The results obtained by modelling and simulation were compared with results obtained experimentally.

Materials descriptors and mechanical properties values, which were used in the verification of the model in design of new steel types and in the researches of mechanical properties of structural steels, were produced by another production company. This data was not used at any stage in the process of building the model.

4. Analysis of own work results

4.1. Results of own work for mechanical properties examination of non alloy and alloy structural steels

The total number of examined melts was 37970. Accepted ranges of investigated steels chemical elements are shown graphically in Fig. 6. Ranges of heat and plastic treatment conditions of examined structural steels are presented on chart Fig. 7a for quenched and tempered steel and on Fig. 7b for normalized steel.
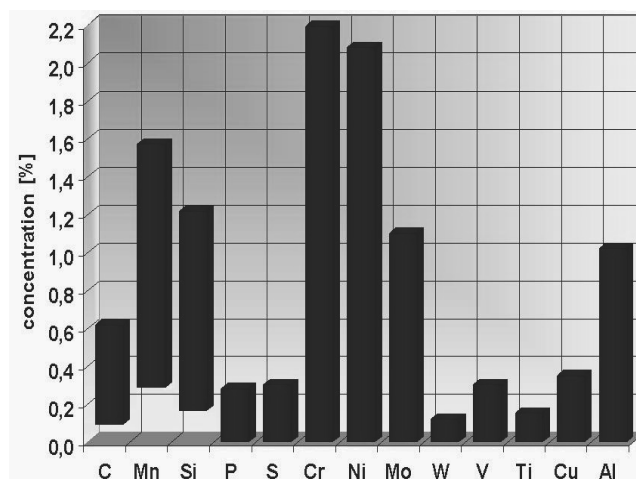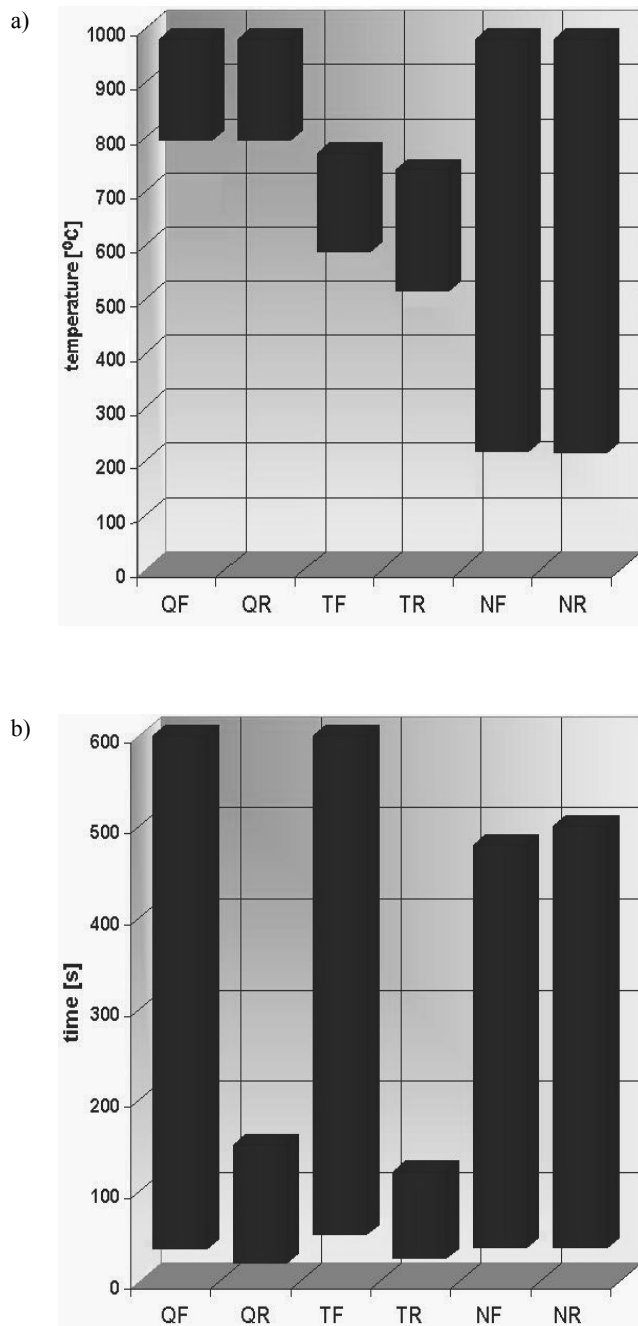

Fig. 6. A chemical elements concentration ranges in investigated structural steels

a)

b)

QF - quenching temperature and time of forged steels,
QR - quenching temperature and time of rolled steels,
TF - tempering temperature and time of forged steels,
TR - tempering temperature and time of rolled steels,
NF - normalising temperature and time of forged steels,
NT - normalising temperature and time of rolled steels,

Fig. 7. Ranges of a) temperature, b) time of heat treatment in investigated structural steels

Materials researches have been partially realised in the laboratories of the Department of Materials Processing Technology, Management and Information Technology in Institute of Engineering Materials and Biomaterials, and partly in a research laboratories "Batory" in Chorzów, Poland [90]. Static steel tensile examinations has been done to determine the yield strength ($R_{0,2}$), tensile strength (R_m), relative elongation (A_5) and relative area reduction (Z). Standard round sample with diameter $\varphi 10$ mm and length 50 mm were used.

The results were divided according to the type of heat and plastic treatment. The chart on Fig. 8a shows results ranges of yield strength $R_{0,2}$, the highest values were found in the case of quenched and tempered steel which the range of 298-1840 MPa. A similar situation exists for tensile strength R_m, where research results are presented in Fig. 8b. Ranges of results for this group of steels are 44-2350 MPa. Values for structural steel after normalisation are much lower and are in the ranges of 208-498 MPa for $R_{0,2}$, and 255-833 MPa for R_m.

Corresponding yield force $F_{0,2}$ and tensile force F_m were calculated from yield strength and tensile strength with appropriate formulas.

Elastic modulus E is also calculated as yield strength divided by the corresponding strain inside the proportional deformation range (below the value of yield strength).

Relative elongation A_5 was designated by comparing the measured sample initial length L_0=50 mm sample with length Lu measured after the break of the samples. The relative area reduction was determined in similar way by comparing the initial sample diameter d_0=10 mm with the smallest cross-section diameter d_u of the sample larger part after the sample's break. The greatest elongation was observed for normalised steel. The results are contained in the range of 10.4-59.8%. For steels after quenching and tempering measured values were much smaller in range of 8.8-39.6%. All results are summarised in Fig. 8c. Designated relative areas reductions are comparable and contains in the range of 34.6-84.5% for steels after quenching and tempering, and in the range of 32.8-78.0% for the normalised steel. Results are introduced in Fig. 8d.

Ranges of impact strength for samples with "V" shape notch (KV) are shown in Fig. 8e, and for samples with "U" shape notch (KCU2) in Fig. 8f. Depending group of steels, the impact strength value were measured in the range of 7-328 J. The smallest variation range was observed for rolled steels after normalisation. For impact strength KCU2 results contained in the range of 9-381J/cm^2 for quenched and tempered steels, and in the range of 33-383J/cm^2 for steels after normalisation. It was noted during researches, that the examination results of samples taken from one rod, with identical chemical composition and identical treatment conditions could be different from each other more then 30%. Therefore, in this research it was decided to give these results in a range between the smallest and the largest value of five independent measurements.

Results of hardness testing are presented in Fig. 8g for Brinell method and in Fig 8h for Vickers method. Quenched and tempered steels have hardness in the range of 123-584 HB and
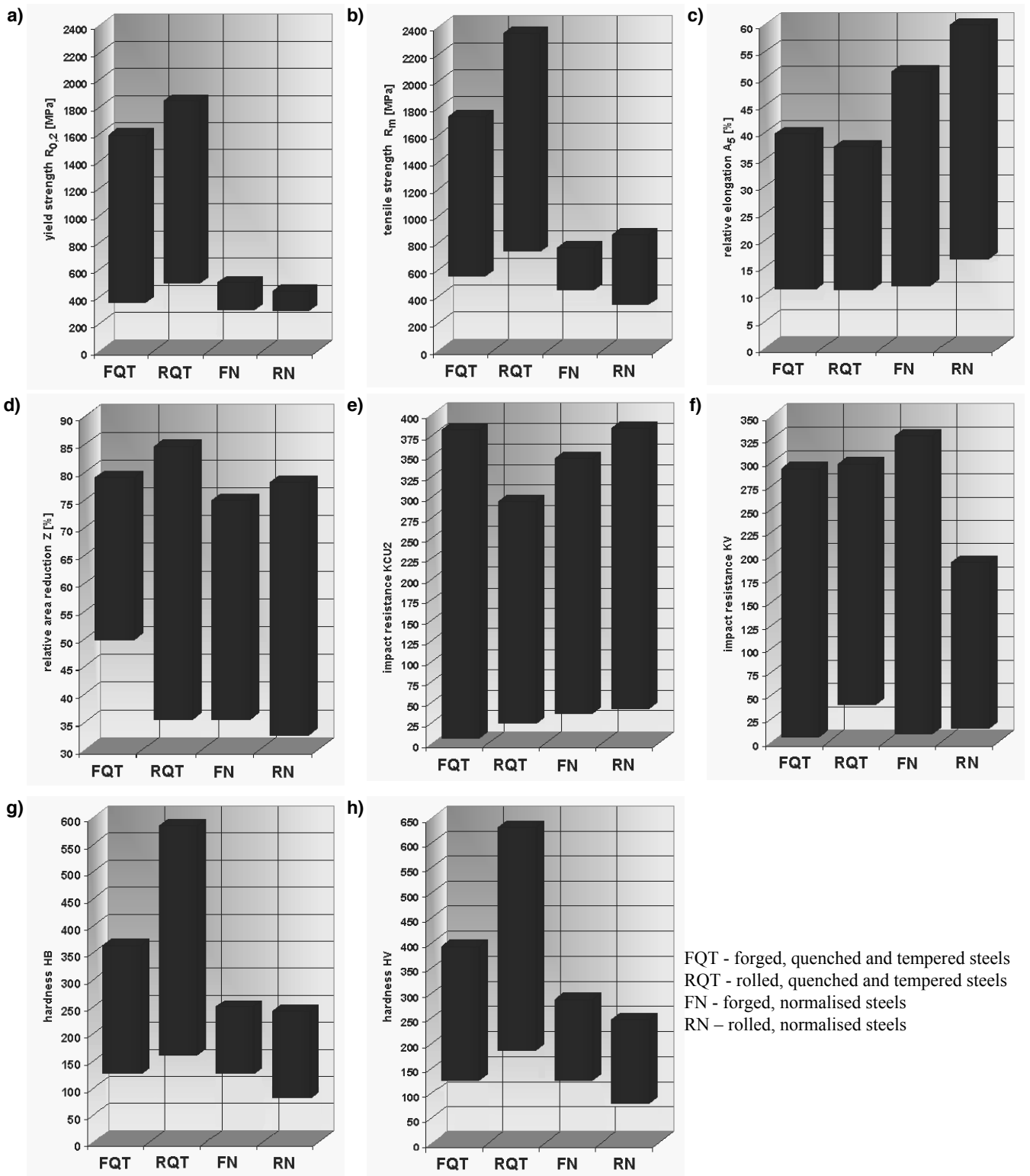
Fig. 8. The ranges of obtained test results a) yield strength $R_{0,2}$, b) tensile strength R_m, c) relative elongation A_5, d) relative area reduction Z, e) impact strength in KV scale, f) impact strength in KCU2 scale, g) Brinell hardness HB, h) Vickers hardness HV

FQT - forged, quenched and tempered steels
RQT - rolled, quenched and tempered steels
FN - forged, normalised steels
RN – rolled, normalised steels

127-630 HV. Much smaller values were obtained for steels after normalisation, respectively 67-249 HB and 66-286 HV. On special attention deserves the similarity in appearance of these two graphs. As in the case of impact strength results, samples taken from this same rod, that means with identical chemical composition and treated under identical conditions, differed from each other, sometimes very significantly. Therefore, in this study it was decided to give the results of hardness in a range between the lowest and highest value of five measurements.

4.2. The results of own work for development of structural steel integrated computational model using artificial neural networks

In order to build the model, set of vectors are divided into four subsets. Division was made because of the differences in

vectors describing steels after heat and plastic treatment. It was decided, that for each individual property, whose value should be estimated, to create a separate neural networks. This applies to the yield strength ($R_{0.2}$), tensile yield strength (R_m), relative elongation (A_5), and relative area reduction (Z). For properties whose values in steel certificates are given in a range, two networks were trained to provide the estimation for the minimum and maximum values separately. This applies to impact strength (KV and KCU2) and hardness (HB and HV). The best results were obtained with artificial neural networks of multilayer perceptron structure with one or two hidden layers. Network types for each property along with the numbers of neurons and the parameters used in quality assessment for a set of test are shown in Table 1.

In all cases, trained artificial neural network reached a value of the correlation coefficient above 0.9 and the relatively low values of deviation ratio. That is a very good representation of the state space. On special attention deserves networks providing

Table 1.
Parameters of computed neural networks for steels after quenching, tempering, normalising, rolling and forging processes

| Properties of forged steel		Quenched and tempered				Normalised			
		Network architecture	average absolute error	standard deviation ratio	Pearson corella-tion	network architecture	average absolute error	standard deviation ratio	Pearson corella-tion
yield strength ($R_{0.2}$)		22:29-9-1:1	26.44	0.20	0.98	18:18-5-1:1	18.14	0.18	0.98
tensile strength (R_m)		22:26-16-13-1:1	23.60	0.19	0.98	18:18-4-1:1	16.02	0.19	0.98
relative elongation (A_5)		17:19-7-1:1	1.26	0.36	0.93	14:14-6-1:1	1.32	0.36	0.93
relative area reduction (Z)		22:26-13-10-1:1	1.7	0.33	0.94	16:16-10-1:1	1.89	0.30	0.95
impact strength (KV)	(min)	16:20-8-1:1	16.42	0.34	0.93	15:15-6-1:1	15.91	0.35	0.93
impact strength (KV)	(max)	24:28-14-1:1	16.64	0.35	0.93	18:18-8-1:1	19.45	0.34	0.93
impact strength (KCU2)	(min)	12:14-7-1:1	10.65	0.35	0.93	14:14-9-1:1	14.62	0.30	0.95
impact strength (KCU2)	(max)	15:17-9-1:1	16.72	0.35	0.93	13:13-8-1:1	14.07	0.24	0.97
Hardness (HB)	(min)	18:22-7-1:1	9.80	0.27	0.96	11:11-5-1:1	4.74	0.29	0.95
Hardness (HB)	(max)	12:16-8-1:1	11.77	0.31	0.94	15:15-6-1:1	6.03	0.33	0.94
Hardness (HV)	(min)	24:28-8-1:1	8.71	0.24	0.97	17:17-7-1:1	6.50	0.32	0.94
Hardness (HV)	(max)	15:19-8-1:1	9.17	0.22	0.97	16:16-4-1:1	6.23	0.33	0.93
Properties of rolled steel		**Quenched and tempered**				**Normalised**			
		Network architecture	average absolute error	standard deviation ratio	Pearson corella-tion	network architecture	average absolute error	standard deviation ratio	Pearson corella-tion
yield strength ($R_{0.2}$)		21:23-26-13-1:1	35.11	0.18	0.98	17:17-9-5-1:1	7.13	0.20	0.98
tensile strength (R_m)		21:23-7-7:1	25.48	0.16	0.98	17:17-12-6-1:1	13.15	0.18	0.98
relative elongation (A_5)		19:21-17-11-1:1	0.97	0.38	0.92	14:14-6-1:1	1.05	0.30	0.95
relative area reduction (Z)		17:19-13-1:1	1.41	0.35	0.93	13:13-4-1:1	1.19	0.31	0.95
impact strength (KV)	(min)	9:9-6-1:1	8.86	0.38	0.92	10:10-5-1:1	20.47	0.41	0.91
impact strength (KV)	(max)	19:21-7-1:1	8.48	0.33	0.94	16:16-6-1:1	19.08	0.37	0.92
impact strength (KCU2)	(min)	17:19-9-1:1	4.91	0.20	0.97	14:14-8-1:1	10.39	0.35	0.93
impact strength (KCU2)	(max)	18:20-8-1:1	6.57	0.26	0.96	16:16-11-1:1	12.16	0.38	0.92
Hardness (HB)	(min)	13:13-8-1:1	8.29	0.29	0.98	8:8-5-1:1	5.84	0.33	0.94
Hardness (HB)	(max)	10:12-6-1:1	8.95	0.22	0.97	12:12-8-1:1	4.76	0.28	0.92
Hardness (HV)	(min)	16:18-12-4-1:1	12.40	0.21	0.97	18:18-8-1:1	5.52	0.33	0.94
Hardness (HV)	(max)	19:19-12-8-1:1	13.94	0.27	0.96	10:10-9-1:1	6.01	0.31	0.94
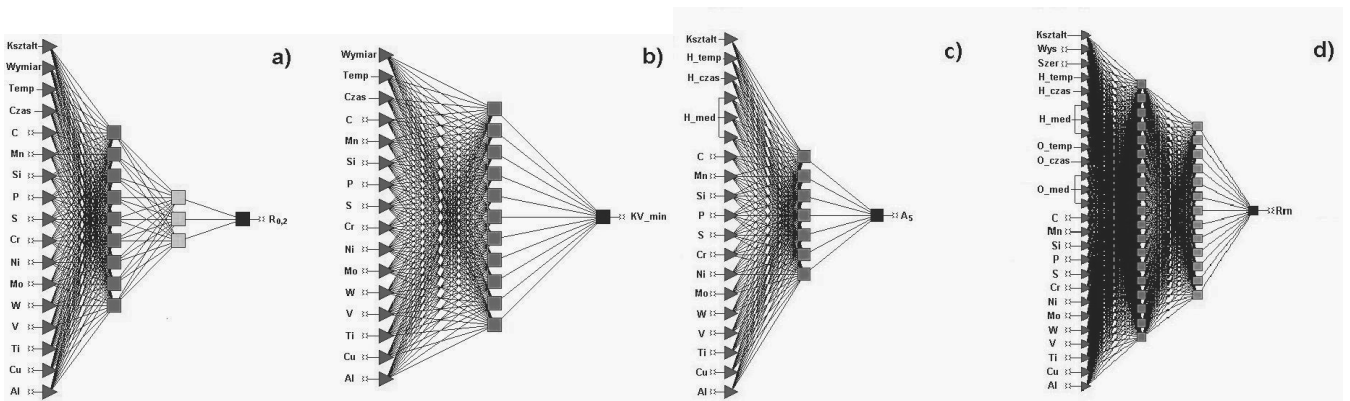
Fig. 9. Architectures of neural net used to prediction of mechanical properties a) yield stress of rolled, normalised steel, four-layer perceptron 17:17-9-3-1:1, b) minimal impact resistance of rolled, normalised steel, three-layer perceptron 16:16-11-1:1, c) relative elongation of forged, quenched and tempered steel, three-layer perceptron 17:19-7-1:1, d) tensile stress of forged, quenched and tempered steel, four-layer perceptron 22:26-16-13-1:1
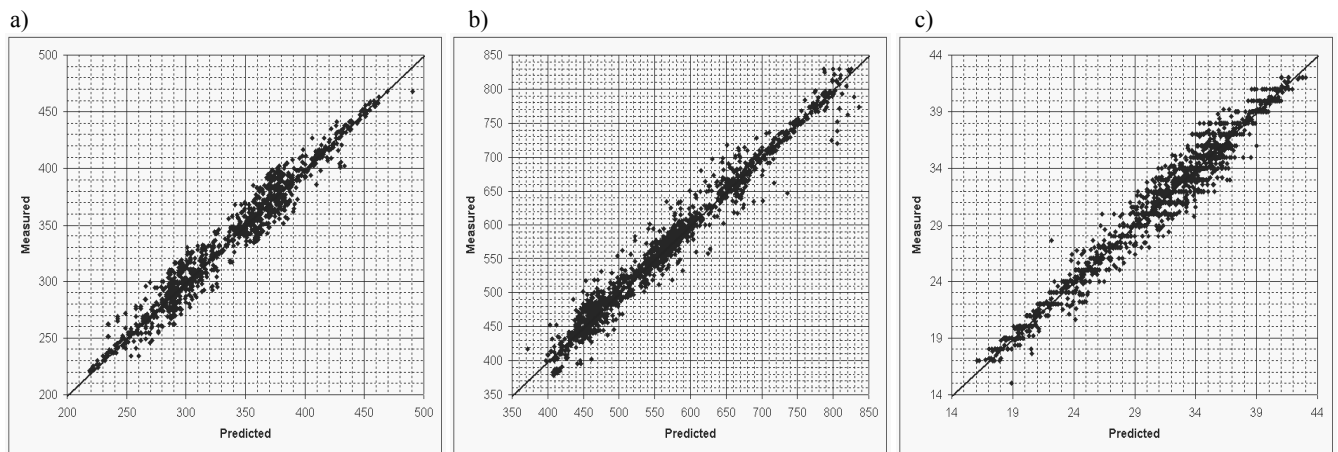

Fig. 10. Examples of comparative graph of a) yield stress R_e, b) strength stress R_m, c) Brinell hardness HB calculated with use of the artificial neural networks and determined experimentally for steels after normalisation

prediction of the yield strength ($R_{0.2}$) and the tensile strength (R_m). The correlation coefficient above 0.98 and the deviation ratio of less than 0.2 indicate a very good network quality. Four of all forty-nine trained networks are shown in Fig. 9.

For graphical illustration of the prediction quality, the Pearson R correlation graphs were developed. They present the comparison between values computed with use of artificial neural network and measured experimentally in real laboratory. For each of the estimated steel's mechanical property vectors distribution is very similar in all three subsets, this proves the correctness of the networks learning processes. Significant differences in the distribution of vectors between groups would imply the possibility of errors, and hence, low quality network. Sample graphs of Person R correlation for a testing subset are shown on Fig. 10.

The developed artificial neural networks were the basis for developing a computational model of structural steel dependences. Block diagram of the model is located in Fig. 11. Forty-eight of the developed artificial neural networks are grouped in four blocks with twelve networks each for steels after

- rolling, quenching and tempering,
- rolling and normalising,
- forging, quenching and tempering,
- forging and normalising,

Appropriate block is activated depending on the type of heat and plastic treatment. Each block contains a set of artificial neural networks necessary to carry out the prediction of mechanical properties. A separate network is responsible for steel's type classifications. The examined steel's concentrations of chemical elements are compared with the chemical concentration of base steels and as a result, a base steel type, which the chemical composition is most similar to examined steel's chemical composition, is given.
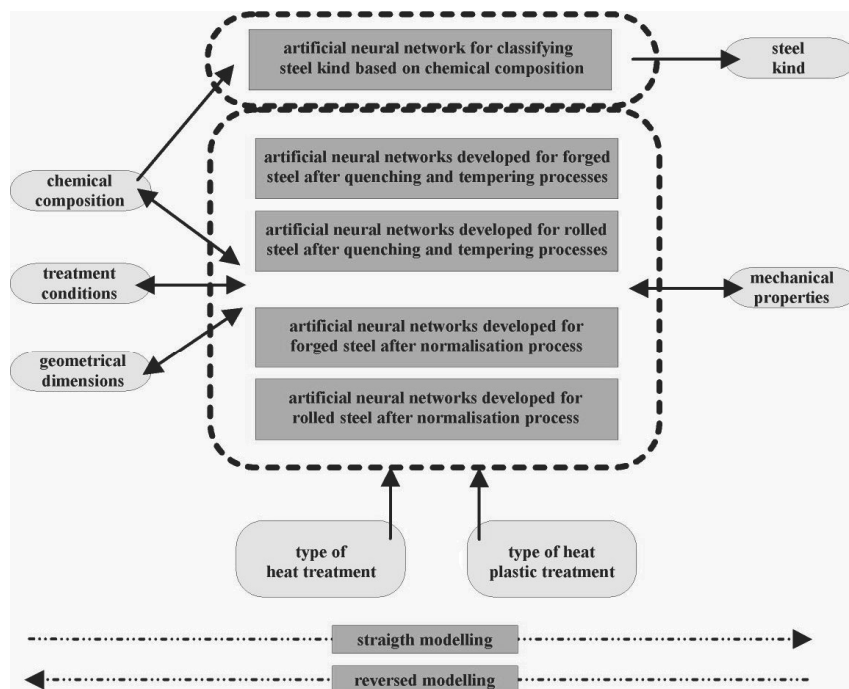
Fig. 11. Block diagram of the developed computational model of properties and descriptors dependencies in structural steel

4.3. The results of own work for development of software for integrated modelling and prediction of mechanical properties

The training of artificial neural networks itself does not make possible the effective prediction of structural steels mechanical parameters. Statistica Neural Network is superb application for training of such networks. However, it is difficult to apply this system as effective environment applicable for properties modelling Necessary becomes the creation of new system, which will:

- use of intuitive graphic user interface,
- protect the user form processing of incorrect data,
- use several neural networks simultaneously in the modelling process,
- make possible the graphic representation of computed results as figures or graphs,
- export the modelling results as raw data or as report,
- allow to save all data as the file on the disc for later use,
- make accessible the necessary documentation, which will enable the beginning of the work to the user and facilitating her guidance.

To fulfil all requirements a material science virtual laboratory has been developed. It is located in the virtual reality an open, academic, research, simulation and teaching environment, which makes possible researches on selected mechanical properties of structural steels.

5. The materials science virtual laboratory project

5.1. The application part of the material science virtual laboratory

The laboratory was divided into two parts with different functionality. The first one is application "NeuroLab" which use artificial intelligence algorithms to predict the mechanical properties of non-alloy and alloy structural steel. It is an application virtual laboratory, in which on the basis of the input steels manufacturing conditions is possible to determine its mechanical properties without the need for real examinations. Also possible is the reversed inference, namely on the basis of mechanical properties values is possible to determine steel's production conditions. The application interface consists of four cards. Input parameters card (Fig. 12a) is used for data input about investigated steel. Predicted results card (Fig. 12b) is used for computation results presentation. Relation chart card (Fig. 12c) is used to generate dependency graphs between the mechanical properties of steel and the production conditions used for their estimation. It is possible to examine the influence of any condition present in input parameters card onto any mechanical property present in predicted results card, when the rest of descriptors remains unchanged. Neural network description card (Fig. 12d) presents information about the

neural networks that were used for the construction of the structural steel dependency model. This model is applied in this software.

The input descriptors are:
- Chemical components:
  - carbon (C),
  - molybdenum (Mn),
  - silicon (Si),
  - phosphorus (P),
  - sulphur (S),
  - chrome (Cr),
  - nickel (Ni),
  - molybdenum (Mo),
  - tungsten (W),
  - vanadium (V),
  - titanium (Ti),
  - copper (Cu),
  - aluminium (Al),
- Mechanical treatment:
  - rolling,
  - forging,
- Heat treatment:
  - quenching and tempering,
    - quenching temperature,
    - quenching time,
    - quenching cooling medium,
    - tempering temperature,
    - tempering time,
    - tempering cooling medium.
- normalisation,
  - normalisation temperature,
  - normalisation time,
  - normalisation cooling medium.
- Shape and size:
  - round (diameter),
  - square (edge size),
  - rectangular (width and height of the rod).

On such basis this programme has the ability to calculate the mechanical properties, such as
- yield force ($F_{0,2}$),
- yield strength ($R_{0,2}$),
- tensile force (F_m),
- tensile strength (R_m),
- elastic modulus (E),
- sample length after examination (L_u),
- relative elongation (A_5),
- sample diameter after examination (d_u),
- relative area reduction (Z),
- impact strength in KV and KCU2 scale,
- hardness in HB and HV scale,
- steel signature.

The results of computational experiments are presented in a openly form in the application window or printed as the investigation protocol of the mechanical and technological properties as print the test protocol of mechanical and technological in accordance with [95]. Relations between production conditions and mechanical properties are generated in the form of graphs in a separate window.
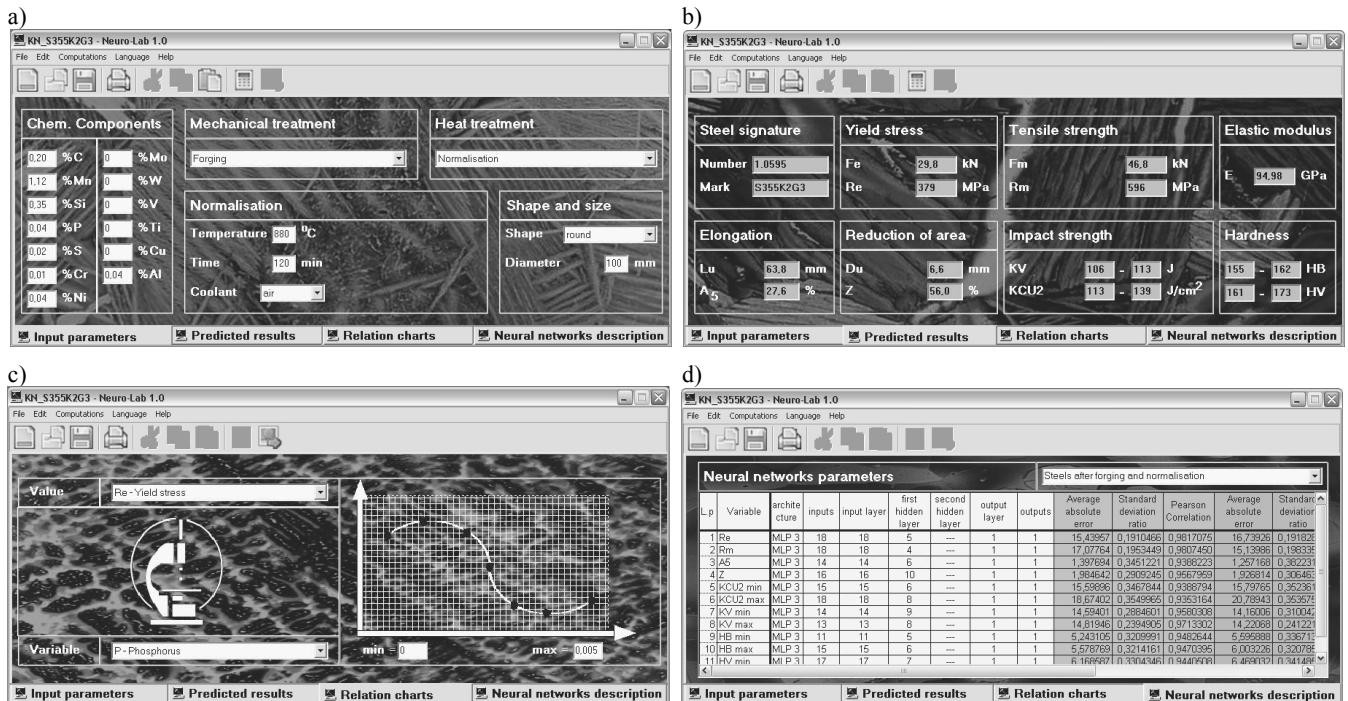

Fig. 12. Application materials science virtual laboratory - NeuroLab 1.1 a) input parameters card, b) predicted results card, c) relation charts card, d) neural networks description card

Fig. 13. Simulation of laboratory equipment installed in network material science virtual laboratory, a) light microscopy, b) laser scanning confocal microscope, c) universal hardness tester, d) scanning electron microscope, e) surface heater, f) tensile machine, g) Charpy pendulum machine, h) samples file generation panel

5.2. The network part of the material science virtual laboratory

Network part of materials science virtual laboratory [92] is a tool with extended functionality in relation to the NeuroLab application. This is a network laboratory placed in the Internet on e-Learning Platform of the Institute of Engineering Materials and Biomaterials. This same computational model of structural steel's dependencies is applied in network part, so it is possible to perform the same examination range, which can be performed using the application part of virtual laboratory. However, there are

differences in examination methodology. Opposite to the application part of the laboratory, in network part user do not receive the results of examinations in the open form. The modelling results are stored in a file, which is a virtual representation of real steel sample in virtual world. In order to obtain the results this file should be placed in machine simulators. Examination of created material model mechanical properties and material structures consists of exact research equipment representation with an exact reproduction of the device's research methodology. Only after the examination performed in the virtual environment, user gets the property examination result (or an error message when the examination failed because of an error).

Figure 13 presents simulations of the investigative equipment available in the laboratory along with the panel for generating files representing material samples.

Network materials science virtual laboratory consists of six workrooms grouped in four laboratories, library and a communication system, that is used to transmit information between students, teachers and instructors present in the workroom. In two workrooms of structure examination laboratory three devices are placed. There are metallographic optical microscope (Fig. 13a), laser scanning confocal microscope (Fig. 13b) and scanning electron microscope (Fig. 13d). In heat treatment laboratory heat is a surface induction heater (Fig. 13e). In two workrooms of material examination laboratories a universal testing machine (Fig. 13f), the universal hardness tester (Fig. 13c) and a Charpy pendulum machine for impact strength examination (Fig. 13g) are placed. In order to perform virtual experiments in the preparation workroom a virtual samples generation panel (Fig. 13h) is installed. It is used to create files representing the materials sample.

Teaching aids are no less important for the processes of active learning from the simulation machines. Properly prepared supporting materials are necessary in the process of research and teaching. Library can be called out by the user trough icons located in each workroom. Communication subsystem consists of a chat-room's is also located in each workroom. It is used to communication between users present at the same time in appropriate workroom. Also available are the bulletin board and a special administrative panel used to express comments and opinions about the functionality and operational of the laboratory.

The research methodology with use of simulations is exactly the same as the real device. All the manipulators, such as buttons or knobs are placed in the simulation at the appropriate places, like in a real machine. The functionality of the real machine is mapped in the simulations without any changes and modifications.

6. The verification of experimental and virtual influence examinations of chemical concentration and conditions of heat and plastic treatment on the mechanical properties of structural steels performed with use of materials science virtual laboratory

In order to experimental verification of computational model successively three aspects has been emerged. The first describes the experimental verifications aimed in the correctness verification of the computational model developed in order to answer the question whether it is possible to perform virtual material examinations exclusively in the virtual environment. This was followed by virtual materials researches aimed to determine the influence, which the structural steel's mechanical properties have on steels descriptors, such as the concentration of chemical elements, the conditions of heat and plastic treatment and geometrical dimensions. The last of these activities was to design a chemical composition and heat treatment conditions of two hypothetical structural steels to meet the client's requirements about values of mechanical properties.

For verification purposes, an experimental set of vectors describing the material descriptors and steel's mechanical properties has been developed. These vectors describe each of the 135 types of examined steel. To exclude the possibility of adjusting the artificial neural network only to the products of one manufacturer's material vectors, verification samples were collected from a different manufacturer. Samples, produced from these types of steel, were examined in order to obtain verification vectors. To minimize differences between training and validation data, material researches has been performed in the same way and using the same equipment, that were used in the main researches. In addition, the vectors used for comparative researches were constructed in the same way as the vectors used for training of artificial neural network used in the calculation model of dependences in to structural steel. Vectors, in which values of material descriptors or mechanical properties went beyond the accepted ranges for the vectors used for construction of artificial neural networks, were rejected. The results obtained by virtual examination have been compared with those obtained experimentally in a real laboratory.

6.1. Influence analysis of admixtures on mechanical properties of structural steels

The influence analysis of the admixtures concentration on the mechanical properties was conducted. Three types of steel were selected for investigations. There are non-alloy structural steels for general use described in [102]. Steel signatures and chemical compositions are introduced in Table 2. The material was delivered as forged, normalised round rods. Delivery conditions are introduced in Table 3. Material descriptors, such as chemical composition, heat treatment, plastic treatment and geometric parameters were inputted to material science virtual laboratory. All data were saved in files, which are representation for real material samples in the virtual world.

The mechanical properties estimation was performed for every single virtual sample. Results obtained with use of this method were compared with results obtained by use of real material investigations. All are introduced in Table 4. It was found, that all estimated results are correct for all examined steel samples, because all three steel species were recognised correctly, and differences among predicted and measured values of mechanical properties are very small and predicted results did not exceed the neural network tolerance values for corresponding property.

NeuroLab system has the ability to generate relation graphs between the mechanical properties of steel and parameters used to

their estimation. Possible is the examination of the influence of any parameter from the input parameters on the value of any mechanical properties from the predicted results, when the rest of parameters remain unchanged.

The next stage of investigative work was the analysis how big is the influence of the admixtures concentration on steels mechanical properties. The influence graphs were generated with use of NeuroLab among estimated properties and the concentration of admixtures. The concentration ranges are:

- Mn to 1.5%,
- Si to 0.5%,
- P to 0.05%,
- S to 0.05%.

Influence graphs are presented in Figs. 14-19.

Table 2.
Chemical composition of examined non-alloy steels

steel signature	C	Mn	Si	P	S	Cr	Ni	Al
S235J2G3	0.16	0.81	0.22	0.01	0.02	0.13	0.09	0.04
S275JR	0.18	0.7	0.31	0.01	0.01	0.11	0.13	0.02
S355K2G3	0.20	1.12	0.35	0.04	0.02	0.01	0.04	0.04

Table 3.
Shape and heat treatment conditions of examined non-alloy steels

steel signature	Normalising			shape
	temperature [°C]	time [min]	cooling medium	
S235J2G3	880	60	Air	Φ100
S275JR	880	60	Air	Φ100
S355K2G3	880	60	Air	Φ100

Table 4.
Comparison between measured and predicted mechanical properties of examined non-alloy steels

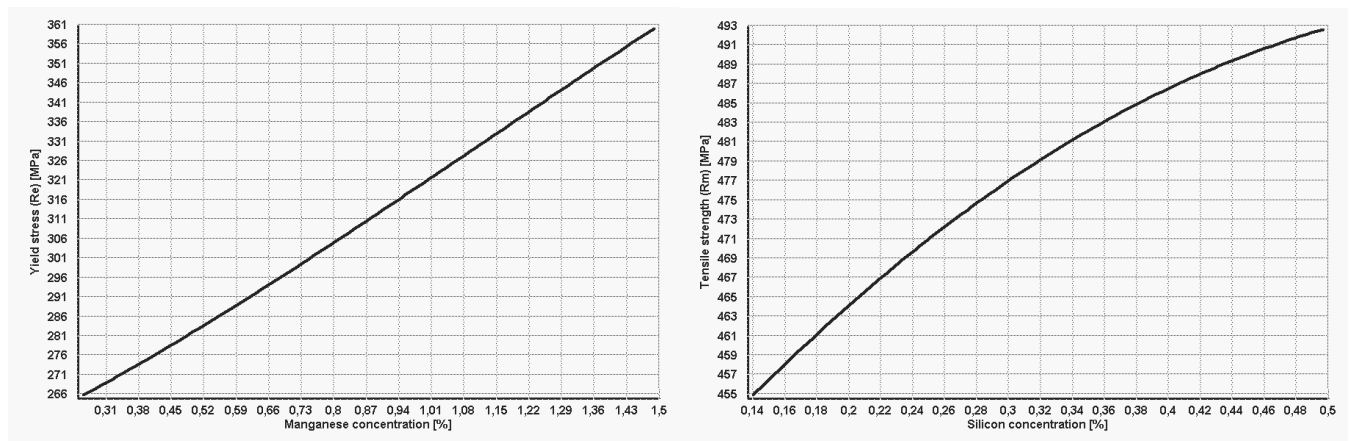| property	measured	predicted	measured	predicted	measured	predicted
Material	S235J2G3	S235J2G3	S275JR	S275JR	S355K2G3	S355K2G3
$R_{0,2}$ [MPa]	307	306	302	304	362	379
R_m [MPa]	461	467	506	502	573	596
A_5 [%]	33.8	34.0	35.5	33.8	31.0	27.6
Z [%]	64.1	65.7	59.9	62.3	52.0	56.0
KV [J]	137-143	108-143	124-142	111-126	102-139	106-113
HB	112-129	124-134	143-146	138-146	149-159	155-162

Fig. 14. Influence of manganese and silicon concentration on selected mechanical properties of S235J2G3 steel
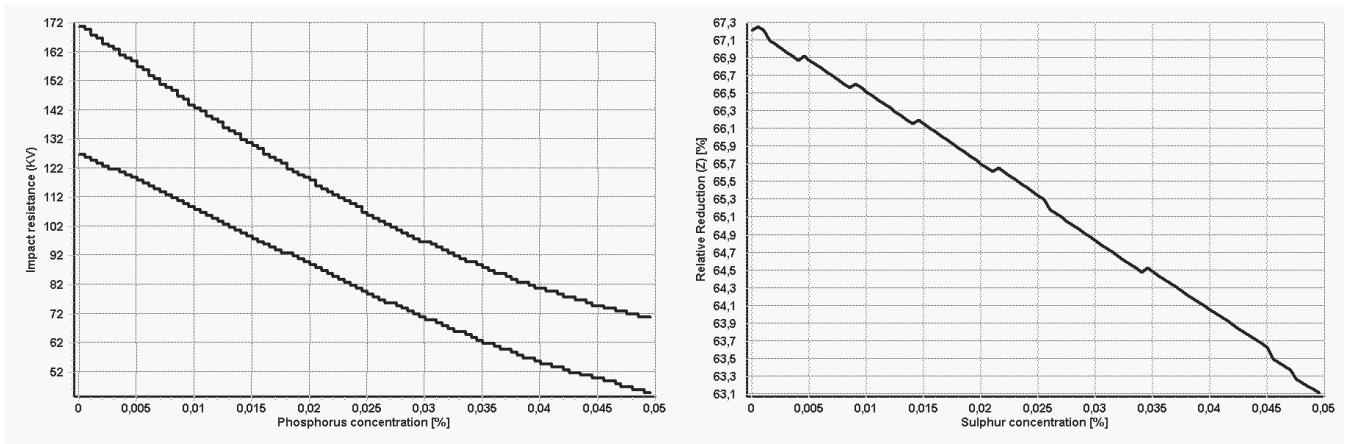
Fig. 15. Influence of phosphorus and sulphur concentration on selected mechanical properties of S235J2G3 steel
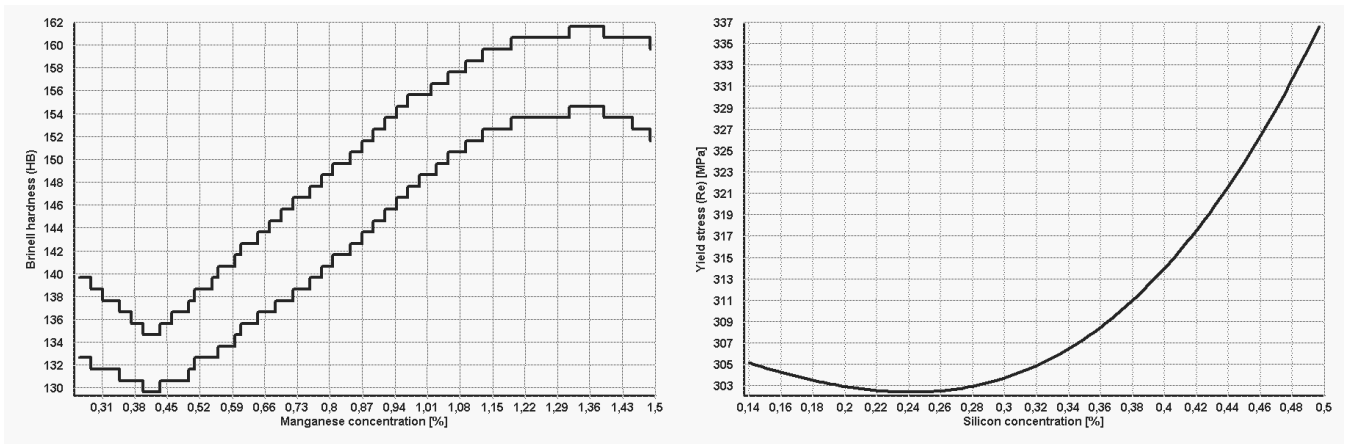

Fig. 16. Influence of manganese and silicon concentration on selected mechanical properties of S275JR steel
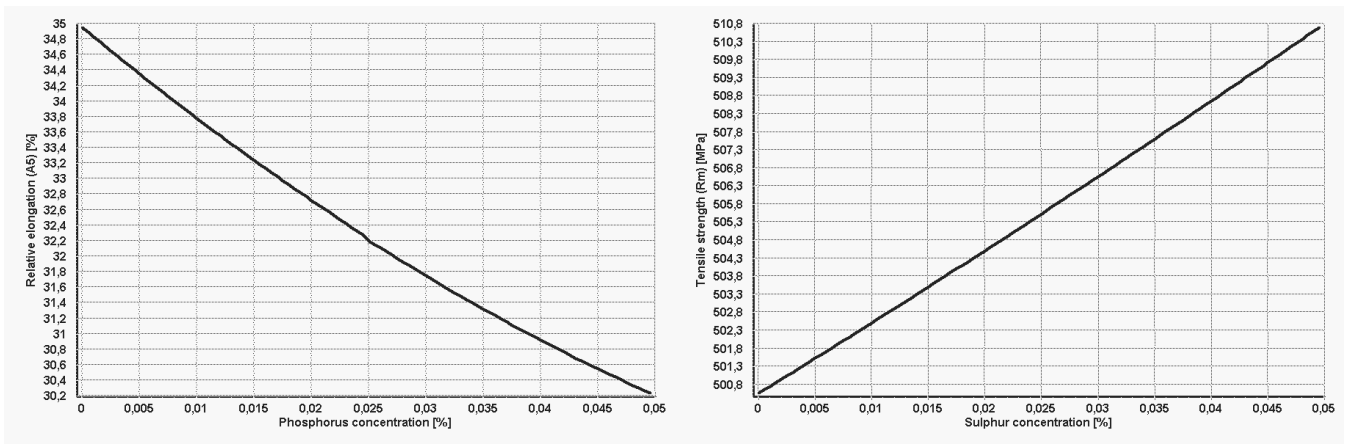

Fig. 17. Influence of phosphorus and sulphur concentration on selected mechanical properties of S275JR steel
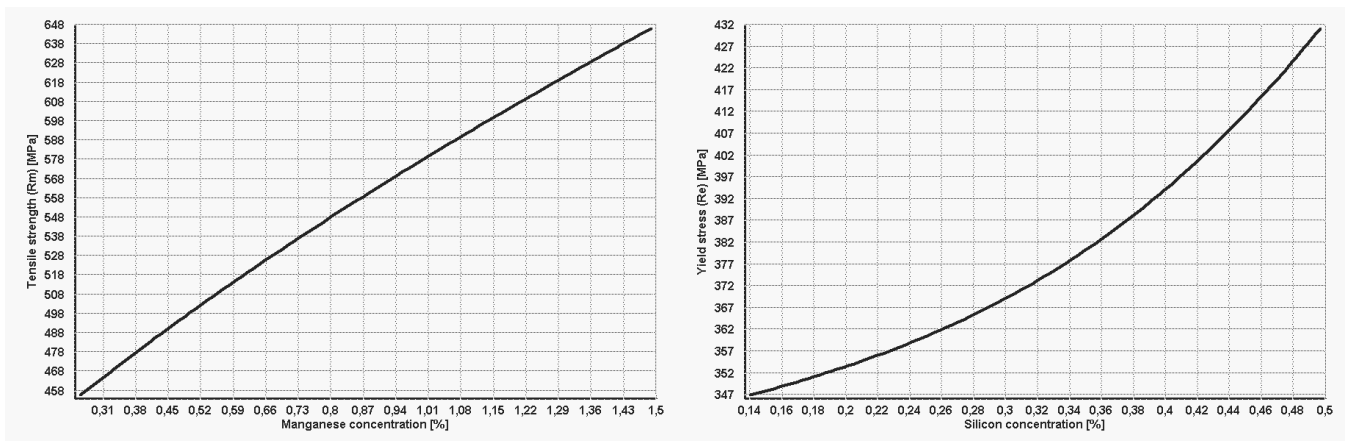
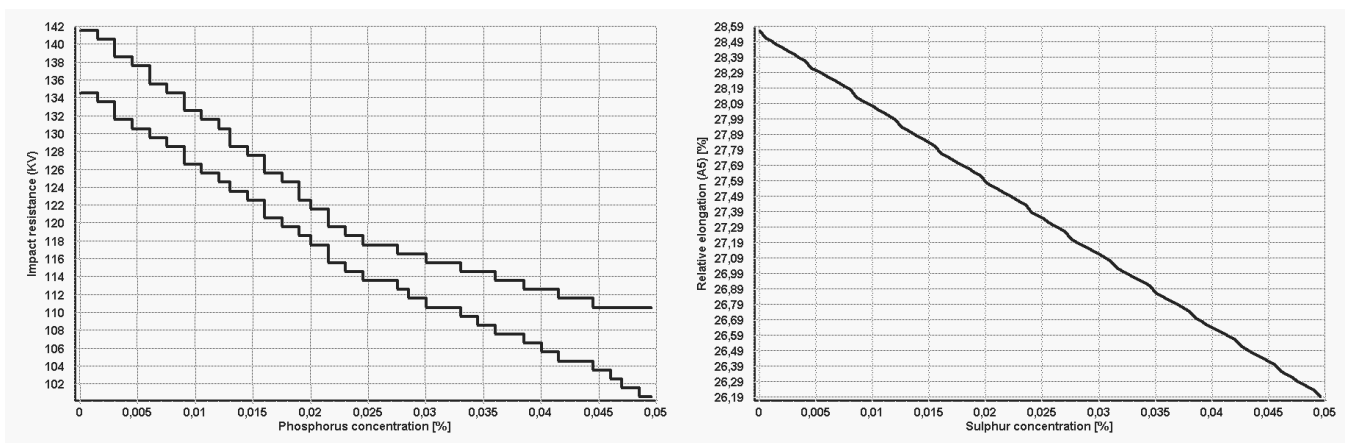Fig. 18. Influence of manganese and silicon concentration on selected mechanical properties of S355K2G3 steel

Fig. 19. Influence of phosphorus and sulphur concentration on selected mechanical properties of S355K2G3 steel

6.2. Influence analysis of alloying additions on mechanical properties of structural steels

Alloy structural steels were the next group of examined materials. Selected were structural steels to toughening produced according to [103]. Alloy additions in these steels are introduced to them by purpose in quantities, which exceeds the given minimum concentration. Steel signatures and the chemical composition of steels selected to examination are introduced in Table 5. Material was delivered as forged round rods. The diameters of rods and heat treatment conditions are introduced in Table 6. In aim of modelling and properties prediction Material descriptors were transferred into materials science virtual laboratory

Results obtained during virtual examinations were compared with the results of real material investigations performed on real steel samples. The mechanical properties prediction was conducted for all selected steel types. Results are introduced in Table 7. Results of modelling were marked as correct, because similarly as with non-alloy steels, all three types were recognised correctly. Differences among measured and predicted values of mechanical properties are very small and the values of the neural networks tolerances were not exceeded. It can be concluded, that results obtained by analysis performed with use of materials science virtual laboratory are correct.

Influence analyses were conducted to calculate how big the influence of the alloy addiction concentration on steels mechanical properties is. Eight alloy addictions were selected - silicon, chrome, molybdenum, tungsten, vanadium, titanium, aluminium and copper. Dependence graphs were generated with use of NeuroLab system among estimated mechanical properties and the concentration of chosen alloying additions. The ranges of concentration were selected above and below the base value. The aim of this was to show how strong the influence is by increasing or decreasing of selected addition chemical concentration on selected mechanical property of examined steels. Selected influence graphs are presented in Figs. 20-25.

Table 5.
Chemical composition of examined alloy steels

steel sign.	C	Mn	Si	P	S	Cr	Ni	Mo	W	V	Ti	Cu	Al
30CrMo5-2	0.33	0.55	0.32	0.014	0.006	2.072	1.24	0.23	0.001	0.02	0.003	0.11	0.024
34CrNiMo6	0.34	0.52	0.2	0.008	0.004	1.48	1.43	0.16	0	0.16	0.001	0.1	0.022
42CrMo4	0.4	0.72	0.24	0.014	0.001	0.99	0.09	0.17	0.001	0.003	0.005	0.13	0.04

Table 6.
Shape and heat treatment conditions of examined alloy steels

steel signature	Quenching			tempering			shape
	temperature [°C]	time [min]	cooling medium	temperature [°C]	time[min]	cooling medium	
30CrMo5-2	860	120	Oil	630	240	air	Φ166
34CrNiMo6	860	150	Polymer	550	240	air	Φ220
42CrMo4	860	120	Water	640	240	air	Φ182

Table 7.
Comparison between measured and predicted mechanical properties of examined alloy steels

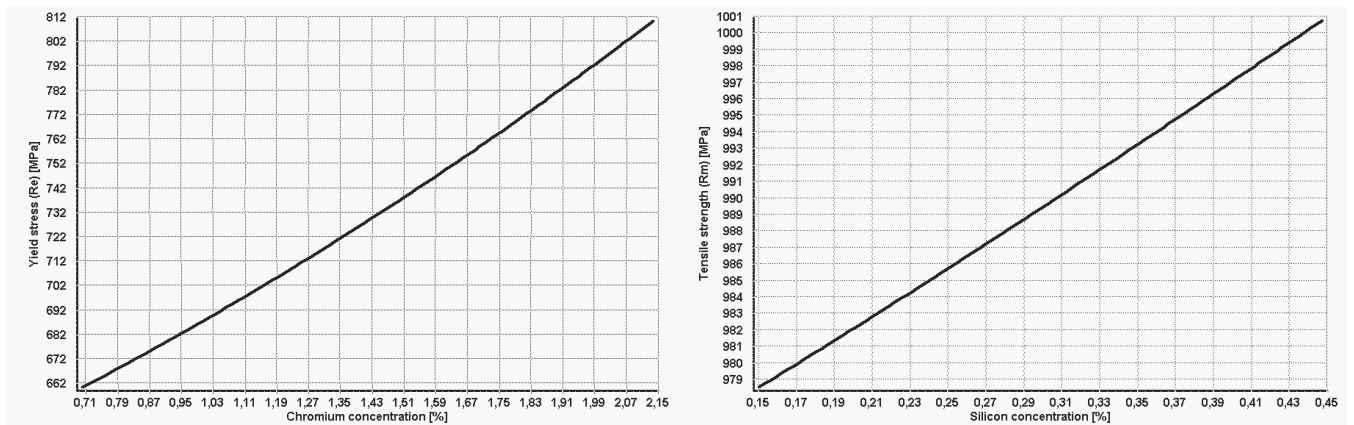| Property	measured	predicted	measured	predicted	measured	predicted
Material	30CrMo5-2	30CrMo5-2	34CrNiMo6	34CrNiMo6	42CrMo4	42CrMo4
$R_{0.2}$ [MPa]	819	803	880	872	616	630
R_m [MPa]	1000	991	976	984	825	851
A_5 [%]	19.6	17.2	15.1	15.2	18.6	18.6
Z [%]	55.1	54.9	52.1	55.6	55.0	55.1
KCU2 [J/cm^2]	76-100	80-112	158-170	155-189	95-130	103-144
HB	277-292	281-289	310-325	316-332	262-269	253-263

Fig. 20. Influence of chromium and silicon concentration on selected mechanical properties of 30CrMo5-2 steel
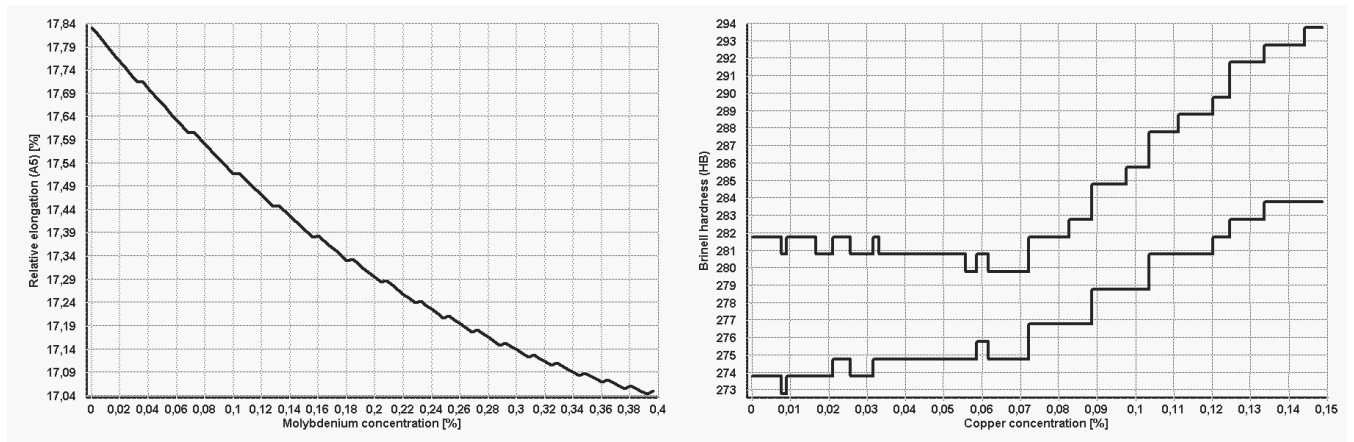

Fig. 21. Influence of molybdenum and copper concentration on selected mechanical properties of 30CrMo5-2 steel
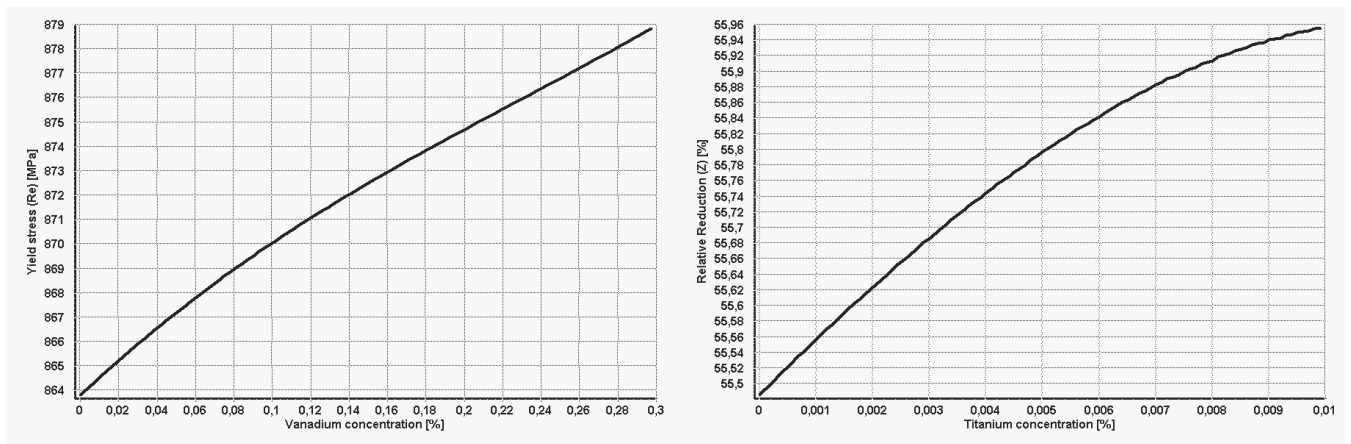
Fig. 22. Influence of vanadium and titanium concentration on selected mechanical properties of 34CrNiMo6 steel
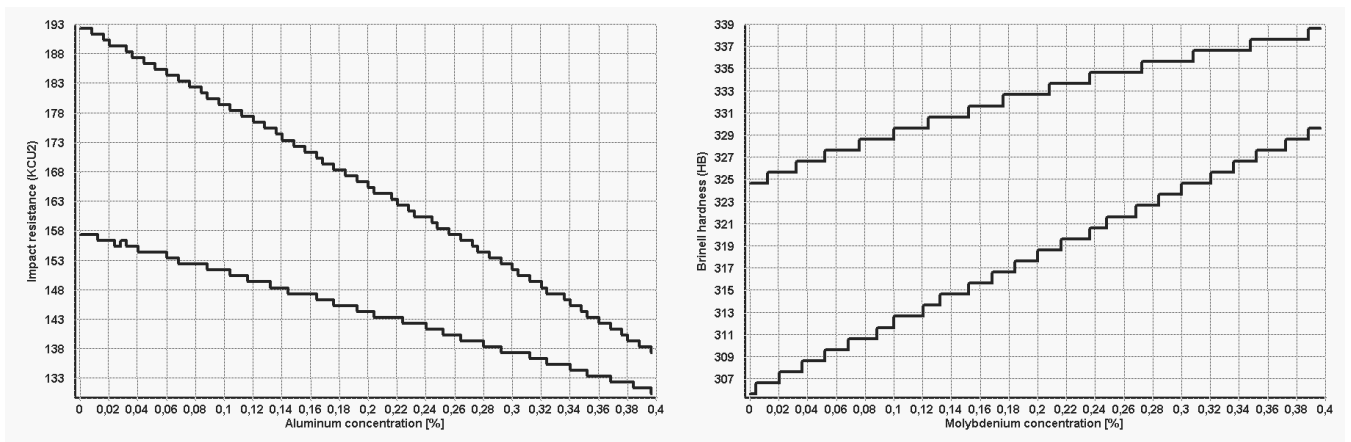

Fig. 23. Influence of aluminium and molybdenum concentration on selected mechanical properties of 34CrNiMo6 steel
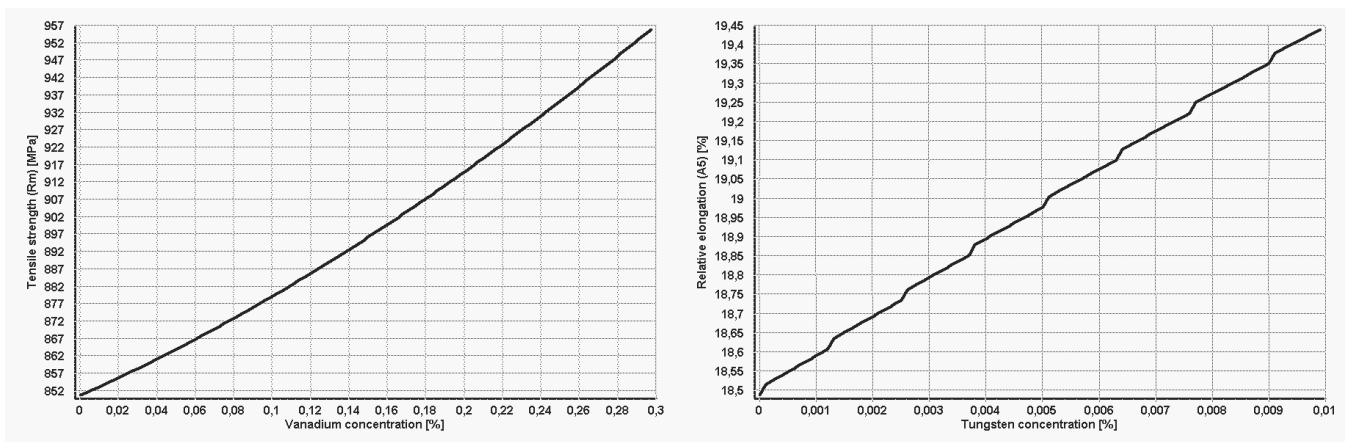

Fig. 24. Influence of vanadium and tungsten concentration on selected mechanical properties of 42CrMo4 steel
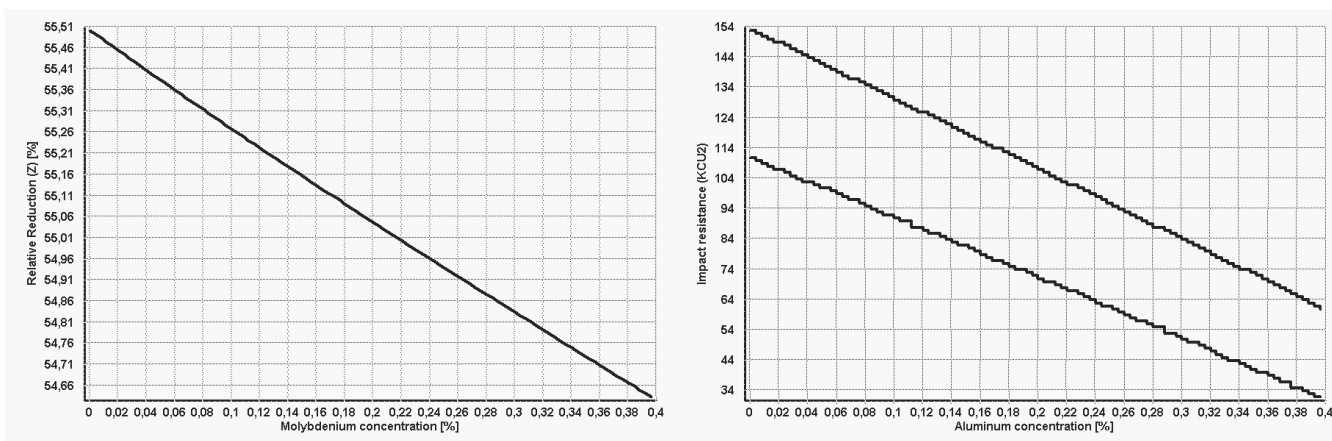
Fig. 25. Influence of molybdenum and aluminium concentration on selected mechanical properties of 42CrMo4 steel

Table 8.
Chemical composition of examined base steels

steel sign	C	Mn	Si	P	S	Cr	Ni	Mo	W	V	Ti	Cu	Al
34CrNiMo6	0.32	0.52	0.16	0.009	0.011	1.48	1.43	0.15	0	0	0	0.19	0
C45R	0.47	0.61	0.39	0.021	0.018	0.31	0.24	0.005	0.002	0.013	0	0.03	0.035

6.3. Results of the virtual designing of new, non standard steel types

The first design task for the virtual science virtual laboratory was to design a steel type, which fulfils the strict delivery conditions for concentrations of chemical elements. Demanded by the virtual client steel chemical composition is presented in Table 8. This is the 34CrNiMo6 steel produced in accordance with [104]. Steel has been heat and plastic treated to appropriate size. Processing conditions and geometric dimensions of the product are introduced in Table 9. Virtual client's demand was that steels chemical composition must be adapted to fulfil strictly defined conditions for the yield strength, tensile strength, relative elongation, impact strength and hardness with unchanged treatment conditions. All given assumptions are summarized in Table 10. For the chemical composition analysis eight chemical elements was selected - carbon, manganese, silicon, chromium, nickel, molybdenum, vanadium and titanium.

The second task was to design virtual steel, which meets strict delivery conditions by modifying only the conditions of heat treatment. Chemical composition of base steel supplied by the client (C45R according to [105]) is given in Table 8. Treatment conditions and geometric dimensions of the product are introduced in Table 9. This time, the virtual client's demand was matching of steel's heat treatment condition. Strictly defined conditions for the yield strength, tensile strength, relative elongation, impact strength and hardness with unchanged chemical composition should be achieved. All assumptions are summarized in Table 10.

Virtual research project in first task consisted in finding such a range of concentrations of given elements, while keeping the other concentrations and treatment conditions unchanged in order to fulfil all conditions for steel properties defined by a virtual client. Virtual research project in the second task included the search for such ranges of temperature and time of quenching and tempering. All conditions for steel properties defined by a virtual client should be fulfilled without changes in the steel's chemical composition.

The results of the analysis are performed in Table 11 for the first task and in Table 13 for the second task. Table 12 shows the results of properties modelling of 34CrNiMo6 steel before and after the modification of chemical composition, Table 14 shows the results of properties modelling of C45R steel before and after the modification of heat treatment conditions. The relative elongation was not included in examinations, because this condition was already fulfilled the base steel.

To verify, if the projecting operations were performed correctly, steels with revisited descriptors have been manufactured in a factory. Steels from both tasks were marked with symbols PR_1 and PR_2. A modified chemical composition of steel is summarized in Table 15, the modified heat treatment conditions of steel PR_2 are summarized in Table 16. Produced steels after heat and plastic treatment were examined in real laboratory. Obtained results are presented together with the results of the virtual examinations performed with use of material science virtual laboratory in Table 17. Real examinations results are comparable with results of virtual examinations, which means, that the projecting operations were performed correctly.

Table 9.
Shape and head treatment conditions of examined base steels

steel signature	Quenching			tempering			shape
	temperature [°C]	time [min]	cooling medium	temperature [°C]	time[min]	cooling medium	
34CrNiMo6	860	180	oil	580	270	air	Φ210
C45R	880	60	oil	690	60	air	Φ100

Table 10.
The required mechanical properties of structural steels for quenching and tempering

Property	34CrNiMo6	C45R
$R_{0.2}$	min. 680 MPa	750-850 MPa
R_m	880-1080 MPa	1200-1320 MPa
A_5	min. 13%	min. 15%
KV	min 40J	min 40 J
HB	277-285	290-300

Table 11.
Results of chemical composition modelling of alloy structural steel for quenching and tempering 34CrNiMo6

property	%C	%Mn	%Si	%Cr	%Ni	%Mo	%V	%Ti
$R_{0.2}$ [MPa]	0.34-0.47	1.01-1.58 *	0.31-0.93	1.68-2.19 *	1.97-2.08 *	0.21-0.89 *	0.02-0.198	--- **
R_m [MPa]	0.35-0.48	0.68-1.47	0.57-1.12	1.25-2.19 *	1.86-2.08 *	0.29-1.09	0.092-0.296	0-0.082
KV_{min} [J]	0.32-0.44	0.26-1.36	0.43-1.20 *	1.24-2.19 *	0-2.01	0-0.53	0-0.3 *	0-0.008
KV_{max} [J]	0.34-0.60 *	0.52-1.58 *	0.14-1.20 *	1.78-2.19 *	0-2.01	0.03-0.49	0.06-0.3 *	0-0.124
HB_{min}	0.38-0.49	1.05-1.48	0.45-0.74	1.86-2.18	--- **	0.55-1.09	0.16-0.3	0.026-0.084
HB_{max}	0.36-0.40	0.92-1.28	0.36-0.54	1.75-2.02	--- **	0.42-0.66	0.094-0.272	0.006-0.012
Range	0.38-0.40	1.05-1.28	---	1.86-2.02	---	---	0.16-0.198	---

* - range of property variability partially exceeded the permissible range of chemical element concentration

** - range of property variability entirely exceeded the permissible range of chemical element concentration

Table 12.
Verification of the mechanical properties of 34CrNiMo6 steel before and after chemical modification

property	not modified	modified C		modified Mn		modified Cr		modified V	
		minimum	maximum	minimum	maximum	Minimum	maximum	minimum	maximum
$R_{0.2}$ [MPa]	660	741	770	684	717	696	712	836	880
R_m [MPa]	910	978	1001	1014	1060	960	981	965	981
A_5 [%]	17.5	16.8	16.6	16.8	16.6	17.7	16.8	16.7	16.5
Z [%]	54.7	54.0	53.8	54.1	54.0	54.7	54.8	54.8	54.9
KV [J]	96-104	78-95	72-92	86-91	85-91	90-99	82-93	82-93	80-91
HB	261-266	278-285	283-292	278-284	285-292	278-292	284-292	278-281	280-284

Table 13.
Results of heat treatment temperature and time modelling of non-alloy structural steel for quenching and tempering C45R

Property	quenching temperature [°C]	quenching time [min]	tempering temperature [°C]	quenching time [min]
$R_{0.2}$ [MPa]	818-877	10-150 *	592-671	61-85
R_m [MPa]	844-887	77-150 *	486-660	86-121
KV_{min} [J]	760-858	63-150	480-740 *	12-120 *
KV_{max} [J]	762-888	41-89	480-740 *	12-120 *
HB_{min}	838-856	10-102 *	589-628	68-76
HB_{max}	848-872	68-150	618-660	62-72
Range	848-856	77-89	658-662	---

* - range of property variability partially exceeded the permissible range of heat treatment temperature or time

Table 14.
Verification of the mechanical properties of C45R steel before and after heat treatment conditions modification

property	not modified	modified quenching temperature		modified quenching time		modified tempering temperature	
		Minimum	Maximum	minimum	Maximum	minimum	maximum
$R_{0.2}$ [MPa]	746	792	779	763	761	817	805
R_m [MPa]	1154	1211	1201	1200	1216	1224	1218
A_5 [%]	21.0	18.5	19.1	19.6	19.4	18.1	18.4
Z [%]	42.7	42.6	42.6	42.7	42.7	41.7	41.7
KV [J]	33-44	43-62	40-58	49-76	58-99	70-92	71-93
HB	279-284	294-300	290-297	292-295	291-294	292-300	290-298

Table 15.
Chemical composition of examined newly designed steels

steel sign.	C	Mn	Si	P	S	Cr	Ni	Mo	W	V	Ti	Cu	Al
PR_1	0.38	0.53	0.17	0.008	0.012	1.49	1.43	0.150	0	0	0	0.19	0.010
PR_2	0.45	0.64	0.39	0.017	0.016	0.30	0.24	0.005	0.002	0.012	0	0.03	0.031

Table 16.
Shape and head treatment conditions of examined newly designed steels

steel signature	Quenching			tempering			shape
	temperature [°C]	time [min]	cooling medium	temperature [°C]	time[min]	cooling medium	
PR_1	860	180	oil	580	270	air	Φ210
PR_2	880	60	oil	690	60	air	Φ100

Table 17.
Comparison between measured and predicted mechanical properties of newly designed steels

property	measured	predicted	measured	predicted
Material	PR_1		PR_2	
$R_{0.2}$ [MPa]	744	748	797	800
R_m [MPa]	980	977	1216	1218
A5 [%]	16.8	16.3	16.7	16.3
Z [%]	54.2	55.1	37.7	36.9
KV [J]	77-94	78-103	96-102	88-113
HB	277-286	280-284	289-296	291-303

7. Summary

On the basis of experimental results obtained in the virtual and real examinations of structural steels mechanical properties it has been proved, that the selection of chemical composition, heat and plastic treatment conditions and geometrical dimensions of structural steels, to ensure the required mechanical properties specified by the designer of machinery and equipment, as the basis for the design of the material elements manufactured from these steels, can be obtain by using a computational model developed using the artificial intelligence tools and virtual environment providing the impact study of these factors on the mechanical properties of steel only in computing environment. Results, obtained during virtual experiments, indicates on very good compatibility of the model with the data obtained experimentally in real laboratory and demonstrate the effectiveness of the model application for the prediction, simulation and modelling of the steel properties and also the design of chemical composition, heat and plastic treatment and geometrical of newly designed steels.

This work is an example of a computational material science, intensively developed in recent years in Institute of Engineering Materials and Biomaterials, Silesian University of Technology, Gliwice, Poland. A virtual research environment built with use of computational model describing relationships between chemical composition, heat and plastic treatment conditions and product geometric dimensions and mechanical properties of the examined group of steel was developed and practical applied. This model enables the design of new structural steels by setting the values of mechanical properties based on material production descriptors and allows the selection of chemical composition, conditions of heat and plastic treatment and geometric dimensions on the basis of the mechanical properties of the product without the need for additional tests and experimental studies in reality.

Described in this paper and implemented in the Institute of Engineering Materials and Biomaterials virtual materials science laboratory met all requirements regarding to enable the conduct of researches in materials science only in the virtual environment. Development of virtual computing environment allows full usage of intelligent dependency model of non-alloy and alloy structural steel properties. This enables the designation of products properties in easy, intuitive and user-friendly way. Also, very easy is the determination of chemical composition, treatment conditions and geometric dimensions of products based on the steels mechanical properties.

The model calculation correctness has been fully verified by experiment. Materials researches performed in the virtual environment, both, in range of determining the mechanical properties and in the field of chemical composition and treatment conditions design, are consistent with the results obtained during the real research in real laboratory. Consistency was observed in the whole range of steel descriptor variation: of concentrations of chemical elements, heat and mechanical treatment conditions and mechanical properties of examined structural steels. Developed virtual environment enables the modelling of new, non-standard types of steel. Through the determination of relations between selected mechanical properties and the steel descriptors at specified range, it is possible to obtain data on the hypothetical and the newly designed materials, which have not been produced yet and existing only in virtual environment. Possibility of designing new materials with unique properties strictly adjusted to actual customer needs is crucial in achieving of the market success.

The proposed solutions allow the usage of developed virtual environment as a new medium in both, the scientific work performed remotely, as well as during classes. It is also possible the extension of developed methodology to other groups of engineering materials, not just steel. The new material design methodology has practical application in the development of materials and modelling of steel descriptors to improve the mechanical properties and specific applications in the production of steel. The presented examples of computer aid in structural steel production showing a potential application possibilities of this methodology to support the production of any group of engineering materials.

Acknowledgements

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